

The Interacting Impurity Josephson Junction: Variational Wavefunctions and Slave Boson Mean Field Theory

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We investigate the Josephson coupling between two superconductors mediated through an infinite U Anderson impurity, adapting a variational wavefunction approach which has proved successful for the Kondo model. Unlike the Kondo problem, however, a crossing of singlet and doublet state energies may be produced by varying the ratio of Kondo energy to superconducting gap, in agreement with recent work of Clerk and Ambegaokar. We construct the phase diagram for the junction and discuss properties of different phases. In addition, we find the singlet and doublet state energies within a slave boson mean field approach. We find the slave boson mean field treatment is unable to account for the level crossing.

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I. INTRODUCTION

The Ambegaokar-Baratoff formula, $I_c = \pi\Delta/2eR$, relates the critical current in a Josephson junction to the superconducting gap Δ and the normal state junction resistance R . This result is perturbative in the electron tunneling amplitude t ; the normal state conductance is proportional to $|t|^2$ when t is small. In certain instances, however, it may be that the tunneling is mediated through a magnetic impurity, rather than taking place directly from one superconductor to the other. This situation has been considered by a number of authors [1–7]. The principal result is that magnetic impurity-mediated tunneling results in a *negative* contribution to I_c . As Kulik originally argued [1], the magnetic impurity gives rise to an effective spin-flip hopping amplitude t_{sf} between the superconductors. Since spin-flip tunneling results in a sign change of the Cooper pair singlet ($\uparrow\downarrow$ to $\downarrow\uparrow$) [5], the critical current is $I_c \propto |t|^2 - |t_{sf}|^2$. When $I_c < 0$, one has a π -junction, for which the ground state energy is minimized when the phase difference between the superconductors is $\delta = \pi$. Such π -junctions break time-reversal symmetry (\mathcal{T}), and a ring containing a single π -junction will enclose trapped flux [3].

This analysis suffices in the perturbative limit where t is small. If the impurity level energy is ε_0 and the Coulomb integral is U , the condition for a magnetic ground state (and a π -junction) is $U > -\varepsilon_0 > 0$ [5]. In the nonperturbative regime, a new energy scale arises: the bare impurity level width $\Gamma \sim \pi\rho|t|^2$, where t is the electrode-impurity hopping matrix element and ρ the electrode density of states. The $T = 0$ phase diagram as a function of $-\varepsilon_0/\Delta$, U/Δ , and Γ/Δ was investigated by the authors [6] within the Hartree-Fock (HF) approximation, where it was found that π -junction behavior occurs for $U > -\varepsilon_0 > 0$, provided Γ is sufficiently small ($\Gamma \lesssim U$). However, when $\Delta = 0$, it is known that the HF approximation is unable to describe the formation of a Kondo

singlet at energy scales below $T_K \equiv W \exp(-\pi|\varepsilon_0|/2\Gamma)$, where W is the half-bandwidth in the electrodes. In our problem, then, one expects that the Kondo effect will be mitigated whenever $\Delta \gtrsim T_K$. Roughly speaking, if $\Delta > T_K$, the ground state of the system is a Kramers doublet, and breaks time reversal symmetry, whereas if $T_K > \Delta$, the ground state is a hybrid singlet formed from electrons on the impurity and in the superconducting electrodes [4].

Recently, Clerk and Ambegaokar [7] applied a generalization of the non-crossing approximation (NCA), a partial summation scheme, to attack this problem in the $U \rightarrow \infty$ limit [7]. Adaptation of this method to the interacting impurity Josephson junction allows one to see a transition from 0-junction to π -junction when the superconducting gap becomes comparable to the Kondo temperature.

In this paper, we also explore the $U \rightarrow \infty$ limit, using two approaches. The first is a variational wave function calculation, similar to that used by Varma and Yafet in the Kondo problem [8,9]. We generalize this wave function in two respects. Firstly, there are two superconductors connected to the impurity. This is in contrast with the usual setup of Kondo problem where we have only metallic electrode. Secondly, the spin- $\frac{1}{2}$ state must be considered as well. We find, in agreement with ref. [7], that a first order transition occurs at $T_K/\Delta \approx 1$. We also show how this transition may be precipitated by a change in the phase difference δ , as we found in ref. [6].

The second calculation we describe is the slave boson mean field theory. While this method does confirm that the singlet state gives a 0-junction and the Kramers doublet a π -junction, within the static slave boson mean field solution the singlet is always lower in energy (or the states are degenerate). The NCA, which goes beyond the mean field level, is able to describe the transition.

II. VARIATIONAL WAVEFUNCTION APPROACH

We start with the grand canonical Hamiltonian $\mathcal{K} \equiv \mathcal{H} - \mu N$,

$$\begin{aligned} \mathcal{K} = \sum_{\alpha} \sum_{\mathbf{q}} \left\{ \xi_{\mathbf{q}\alpha} (\psi_{\mathbf{q}\alpha\uparrow}^\dagger \psi_{\mathbf{q}\alpha\uparrow} + \psi_{\mathbf{q}\alpha\downarrow}^\dagger \psi_{\mathbf{q}\alpha\downarrow}) \right. \\ + \Delta_{\alpha} \left(e^{i\delta_{\alpha}} \psi_{\mathbf{q}\alpha\uparrow}^\dagger \psi_{-\mathbf{q}\alpha\downarrow}^\dagger + e^{-i\delta_{\alpha}} \psi_{-\mathbf{q}\alpha\downarrow}^\dagger \psi_{\mathbf{q}\alpha\uparrow} \right) \\ - \frac{1}{\sqrt{\mathcal{N}_{\alpha}}} \sum_{\sigma=\uparrow,\downarrow} \left(t_{\alpha} \psi_{\mathbf{q}\alpha\sigma}^\dagger c_{\sigma} + t_{\alpha}^* c_{\sigma}^\dagger \psi_{\mathbf{q}\alpha\sigma} \right) \Big\} \\ \left. + \varepsilon_0 (c_{\uparrow}^\dagger c_{\uparrow} + c_{\downarrow}^\dagger c_{\downarrow}) + U c_{\uparrow}^\dagger c_{\downarrow}^\dagger c_{\downarrow} c_{\uparrow} \right\}, \quad (1) \end{aligned}$$

where α labels the electrode, $\xi_{\mathbf{q}\alpha}$ is the dispersion in the α electrode relative to the chemical potential, Δ_{α} is the modulus of the superconducting gap and δ_{α} its phase, \mathcal{N}_{α} is the number of unit cells in electrode α , t_{α} is the hopping amplitude from electrode α to the impurity, and ε_0 is the bare impurity energy. We set $U \rightarrow \infty$, which leads to the constraint $\sum_{\sigma} c_{\sigma}^\dagger c_{\sigma} \leq 1$.

Defining the angle $\theta_{\mathbf{q}\alpha} \equiv \tan^{-1}(\Delta_{\alpha}/\xi_{\mathbf{q}\alpha})$ and the usual BCS coherence factors $u_{\mathbf{q}\alpha} = \cos(\frac{1}{2}\theta_{\mathbf{q}\alpha})$, $v_{\mathbf{q}\alpha} = \sin(\frac{1}{2}\theta_{\mathbf{q}\alpha}) \exp(i\delta_{\alpha})$, we express $\mathcal{K} = \mathcal{K}_0 + \mathcal{K}_1$ in terms of the Bogoliubov quasiparticle operators:

$$\begin{aligned} \mathcal{K}_0 = \sum_{\mathbf{q}, \alpha} E_{\mathbf{q}\alpha} (\gamma_{\mathbf{q}\alpha\uparrow}^\dagger \gamma_{\mathbf{q}\alpha\uparrow} + \gamma_{\mathbf{q}\alpha\downarrow}^\dagger \gamma_{\mathbf{q}\alpha\downarrow}) + \varepsilon_0 (c_{\uparrow}^\dagger c_{\uparrow} + c_{\downarrow}^\dagger c_{\downarrow}) \\ + U c_{\uparrow}^\dagger c_{\downarrow}^\dagger c_{\downarrow} c_{\uparrow} \\ \mathcal{K}_1 = \sum_{\mathbf{q}, \alpha} t_{\mathbf{q}\alpha} \left\{ u_{\mathbf{q}\alpha} (\gamma_{\mathbf{q}\alpha\uparrow}^\dagger c_{\uparrow} + \gamma_{\mathbf{q}\alpha\downarrow}^\dagger c_{\downarrow} + c_{\uparrow}^\dagger \gamma_{\mathbf{q}\alpha\uparrow} + c_{\downarrow}^\dagger \gamma_{\mathbf{q}\alpha\downarrow}) \right. \\ \left. + v_{\mathbf{q}\alpha} (\gamma_{\mathbf{q}\alpha\uparrow}^\dagger c_{\downarrow}^\dagger - \gamma_{\mathbf{q}\alpha\downarrow}^\dagger c_{\uparrow}^\dagger) + v_{\mathbf{q}\alpha}^* (\gamma_{\mathbf{q}\alpha\downarrow} c_{\uparrow} - \gamma_{\mathbf{q}\alpha\uparrow} c_{\downarrow}) \right\}, \end{aligned}$$

where $E_{\mathbf{q}\alpha} = \sqrt{\xi_{\mathbf{q}\alpha}^2 + \Delta_{\alpha}^2}$, and $t_{\mathbf{q}\alpha} \equiv |t_{\alpha}|/\sqrt{\mathcal{N}_{\alpha}}$.

We now two variational many-body states for the $U = \infty$ limit: a singlet,

$$\begin{aligned} |\text{S}\rangle \equiv \left\{ A + \sum_{\mathbf{q}, \alpha} \frac{1}{\sqrt{2}} B_{\mathbf{q}\alpha} (\gamma_{\mathbf{q}\alpha\uparrow}^\dagger c_{\downarrow} - \gamma_{\mathbf{q}\alpha\downarrow}^\dagger c_{\uparrow}^\dagger) \right. \\ \left. + \sum_{\mathbf{q}'\alpha'} C_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'} \gamma_{\mathbf{q}\alpha\uparrow}^\dagger \gamma_{\mathbf{q}'\alpha'\downarrow}^\dagger \right\} |0\rangle, \quad (2) \end{aligned}$$

and a doublet,

$$\begin{aligned} |\text{D}\uparrow\rangle \equiv \left\{ \tilde{A} c_{\uparrow}^\dagger + \sum_{\mathbf{q}, \alpha} \tilde{B}_{\mathbf{q}\alpha} \gamma_{\mathbf{q}\alpha\uparrow}^\dagger + \sum_{\mathbf{q}, \alpha} \left[\tilde{C}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'} \gamma_{\mathbf{q}\alpha\uparrow}^\dagger \gamma_{\mathbf{q}'\alpha'\downarrow}^\dagger c_{\uparrow}^\dagger \right. \right. \\ \left. \left. + \frac{1}{\sqrt{3}} \tilde{D}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'} (\gamma_{\mathbf{q}\alpha\uparrow}^\dagger \gamma_{\mathbf{q}'\alpha'\downarrow}^\dagger c_{\uparrow}^\dagger - \gamma_{\mathbf{q}\alpha\uparrow}^\dagger \gamma_{\mathbf{q}'\alpha'\uparrow}^\dagger c_{\downarrow}^\dagger) \right] \right\} |0\rangle, \quad (3) \end{aligned}$$

where $|0\rangle$ is the fermion vacuum (the other doublet state $|\text{D}\downarrow\rangle$ is obtained by rotating the spins by π about the

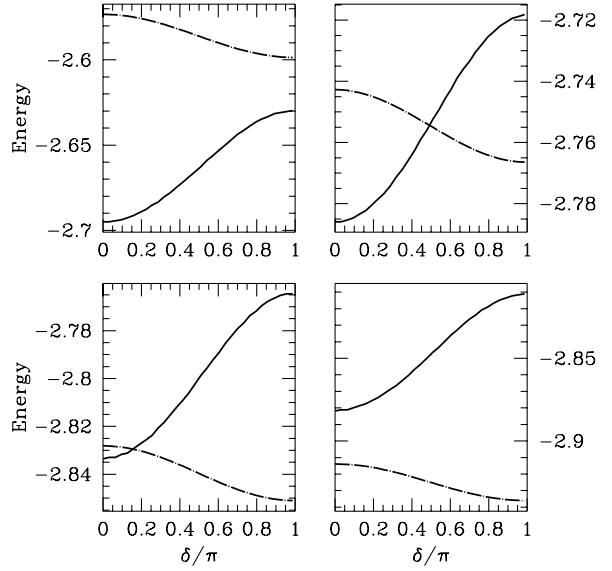


FIG. 1. Singlet (solid) and doublet (dot-dash) energies versus phase difference for $\varepsilon_0 = -1.6$ (upper left), $\varepsilon_0 = -1.8$ (upper right), $\varepsilon_0 = -1.9$ (lower left), and $\varepsilon_0 = -2.0$ (lower right). In all cases $\Delta = 1$ and $\Gamma_L = \Gamma_R = 0.3\pi$.

y -axis). Here, $C_{\mathbf{q}'\mathbf{q}}^{\alpha'\alpha} = C_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$, $\tilde{C}_{\mathbf{q}'\mathbf{q}}^{\alpha'\alpha} = \tilde{C}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$, and $\tilde{D}_{\mathbf{q}'\mathbf{q}}^{\alpha'\alpha} = -\tilde{D}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$. We next set to zero the variations

$$\delta \langle \Psi | \mathcal{K}_0 + \mathcal{K}_1 | \Psi \rangle - E \delta \langle \Psi | \Psi \rangle = 0, \quad (4)$$

where $|\Psi\rangle$ is $|\text{S}\rangle$ or $|\text{D}\uparrow\rangle$, to obtain equations relating the variational coefficients. We find that A and the matrix $C_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$ may be expressed in terms of the coefficients $B_{\mathbf{q}\alpha}$, and similarly \tilde{A} and the matrices $\tilde{C}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$ and $\tilde{D}_{\mathbf{q}\mathbf{q}'}^{\alpha\alpha'}$ may be expressed in terms of the coefficients $\tilde{B}_{\mathbf{q}\alpha}$. We then obtain the two eigenvalue equations for the singlet and doublet energies E and \tilde{E} , respectively:

$$\begin{aligned} \sum_{\mathbf{q}'\alpha'} \left[\frac{2 v_{\mathbf{q}\alpha} v_{\mathbf{q}'\alpha'}^* t_{\mathbf{q}\alpha} t_{\mathbf{q}'\alpha'}}{E} + \frac{u_{\mathbf{q}\alpha} u_{\mathbf{q}'\alpha'} t_{\mathbf{q}\alpha} t_{\mathbf{q}'\alpha'}}{E - E_{\mathbf{q}\alpha} - E_{\mathbf{q}'\alpha'}} \right] B_{\mathbf{q}'\alpha'} \\ = \left[E - E_{\mathbf{q}\alpha} - \varepsilon_0 - \sum_{\mathbf{q}',\alpha'} \frac{u_{\mathbf{q}'\alpha'}^2 t_{\mathbf{q}'\alpha'}^2}{E - E_{\mathbf{q}\alpha} - E_{\mathbf{q}'\alpha'}} \right] B_{\mathbf{q}\alpha} \quad (5) \end{aligned}$$

and

$$\begin{aligned} \sum_{\mathbf{q}'\alpha'} \left[\frac{u_{\mathbf{q}\alpha} u_{\mathbf{q}'\alpha'} t_{\mathbf{q}\alpha} t_{\mathbf{q}'\alpha'}}{\tilde{E} - \varepsilon_0} + \frac{v_{\mathbf{q}\alpha} v_{\mathbf{q}'\alpha'}^* t_{\mathbf{q}\alpha} t_{\mathbf{q}'\alpha'}}{\tilde{E} - \varepsilon_0 - E_{\mathbf{q}\alpha} - E_{\mathbf{q}'\alpha'}} \right] \tilde{B}_{\mathbf{q}'\alpha'} \\ = \left[\tilde{E} - E_{\mathbf{q}\alpha} - \sum_{\mathbf{q}',\alpha'} \frac{2|v_{\mathbf{q}'\alpha'}|^2 t_{\mathbf{q}'\alpha'}^2}{\tilde{E} - \varepsilon_0 - E_{\mathbf{q}\alpha} - E_{\mathbf{q}'\alpha'}} \right] \tilde{B}_{\mathbf{q}\alpha} \quad (6) \end{aligned}$$

We solve these equations numerically for the symmetric case $\Delta_L = \Delta_R = \Delta$, $t_L = t_R = t$, $\Gamma_L = \Gamma_R = \Gamma$. The normal state of each electrode is described by a flat band of width $2W$; we use $W/\Delta = 10$ in our calculations, but the general features are rather insensitive to the value of

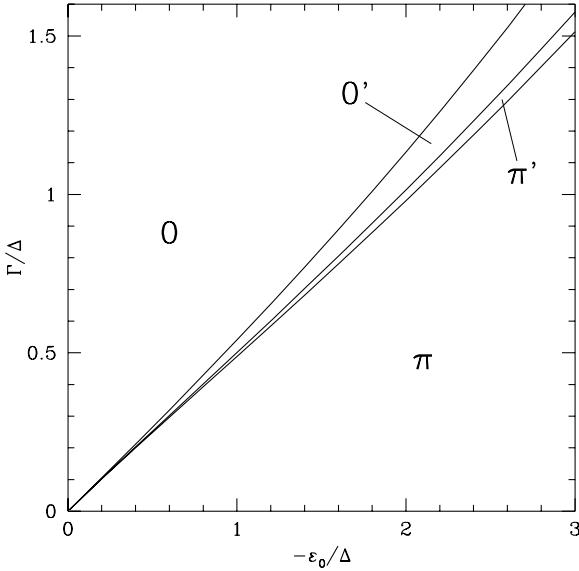


FIG. 2. Variational wavefunction phase diagram for the symmetric case $\Gamma_L = \Gamma_R \equiv \Gamma$.

W . Energy *versus* phase difference, $E(\delta)$, is plotted in figure 1 for $\Delta = 1$, $\Gamma = 0.3\pi$, for four different values of $-\varepsilon_0$. When $\varepsilon_0 = -1.6$, the singlet state is the ground state for all δ , while for $\varepsilon_0 = -2.0$, the ground state is always the doublet. These are 0- and π -junctions, respectively. For $\varepsilon_0 = -1.8$, the curves cross, and the ground state energy has a kink as a function of δ . Both $\delta = 0$ and $\delta = \pi$ are local minima in $E(\delta)$, with $\delta = 0$ the global minimum. Using the terminology of ref. [6], this is a $0'$ -junction. The final case of the π' -junction is reflected in the curves for $\varepsilon_0 = -1.9$, where $\delta = 0$ is a local minimum and $\delta = \pi$ the global minimum of the energy.

The phase diagram is displayed in fig. 2. In the HF treatment [6], one also finds a transition from π to π' to $0'$ to 0-junction phases as Γ is increased from zero. However, the critical value of Γ there turns out to be inversely proportional to $\ln U$. There are two reasons for this: first, the HF calculations assumed an infinite bandwidth, and second, HF is unable to describe the formation of a Kondo singlet. Here, the transition from 0-junction to π -junction occurs roughly for $\Delta \sim T_K$, in agreement with ref. [7]. Indeed, when $0 < -\varepsilon_0, \Gamma \ll \Delta$ this relation can be derived within perturbation theory. The perturbative value of energy of the singlet state is

$$E_0 \approx -\frac{4\Gamma}{\pi} \ln \frac{2W}{\Delta}, \quad (7)$$

while the energy of the doublet is

$$E_\uparrow \approx \varepsilon_0 - \frac{2\Gamma}{\pi} \ln \frac{2W}{\Delta}. \quad (8)$$

Comparing these two we find that the symmetry of the ground state changes when

$$\Delta = 2W \exp(-\pi|\varepsilon_0|/2\Gamma) = 2T_K. \quad (9)$$

This predicts a straight line for Γ *versus* $-\varepsilon_0$ with a slope $\Gamma/(-\varepsilon_0) = \pi/2 \ln(2W/\Delta)$. With $W = 10\Delta$, the slope is 0.524, and the line would be bounded by the $0 - 0'$ and $\pi - \pi'$ phase boundaries in fig. 2 (it is not shown for the purposes of clarity).

III. SLAVE BOSON MEAN FIELD THEORY

We consider an extension of the model of eqn. (1) by introducing a flavor -1 m which runs from 1 to N_f . The Hamiltonian is then

$$\begin{aligned} \mathcal{K} = & \sum_{\alpha} \sum_{m=1}^{N_f} \sum_{\mathbf{q}} \left\{ \sum_{\sigma=\uparrow,\downarrow} (\xi_{\mathbf{q}\alpha} + \mu_B B \sigma) \psi_{\mathbf{q}\alpha m\sigma}^\dagger \psi_{\mathbf{q}\alpha m\sigma} + \right. \\ & \Delta_\alpha \left(e^{i\delta_\alpha} \psi_{\mathbf{q}\alpha m\uparrow}^\dagger \psi_{-\mathbf{q}\alpha m\downarrow}^\dagger + e^{-i\delta_\alpha} \psi_{-\mathbf{q}\alpha m\downarrow} \psi_{\mathbf{q}\alpha m\uparrow} \right) \\ & - \frac{1}{\sqrt{N_\alpha}} \sum_{\sigma=\uparrow,\downarrow} \left(t_\alpha \psi_{\mathbf{q}\alpha m\sigma}^\dagger c_{m\sigma} + t_\alpha^* c_{m\sigma}^\dagger \psi_{\mathbf{q}\alpha m\sigma} \right) \Big\} \\ & + \sum_{m=1}^{N_f} \sum_{\sigma=\uparrow,\downarrow} (\varepsilon_0 + \mu_B B \sigma) c_{m\sigma}^\dagger c_{m\sigma}, \end{aligned} \quad (10)$$

where $\mu_B B$ is the Zeeman energy. The impurity level occupancy satisfies the constraint $\sum_{m,\sigma} c_{m\sigma}^\dagger c_{m\sigma} \leq r$. We refer to this as model I. In a slightly different large- N_f extension (model II), we rescale the hopping amplitudes $t_\alpha \rightarrow t_\alpha/\sqrt{N_f}$ and write the constraint as $\sum_{m,\sigma} c_{m\sigma}^\dagger c_{m\sigma} \leq r N_f$. In both cases, $0 \leq r \leq 2$.

Introducing a slave boson b and a Lagrange multiplier λ to impose the constraint, we evaluate the impurity contribution to the free energy at the mean field level, assuming both b and λ to be static. The impurity free energy per flavor is then

$$\begin{aligned} F_{\text{imp}}/N_f = & \varepsilon - \mu_B B + p(\varepsilon - \varepsilon_0)(|b|^2 - r) \\ & + \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega + \mu_B B) \text{Im} \ln H(\omega + i0^+) \\ H(\omega) = & \omega^2 - \varepsilon^2 - (2|b|^2 \Gamma_a)^2 + \frac{\left[2|b|^2 \Gamma_g \Delta \sin\left(\frac{1}{2}\delta\right) \right]^2}{\Delta^2 - \omega^2} \\ & + \frac{4|b|^2 \Gamma_a \omega^2}{\sqrt{\Delta^2 - \omega^2}} \end{aligned} \quad (11)$$

where $\Gamma_a = \frac{1}{2}$, $\Gamma_g = \sqrt{\Gamma_L \Gamma_R}$ with $\Gamma_\alpha = \pi \rho_\alpha |t_\alpha|^2$ (ρ_α is the bare density of states per unit cell in electrode α), $\delta = \delta_L - \delta_R$ is the phase difference between the two superconducting electrodes (we assume $\Delta_1 = \Delta_2 \equiv \Delta$), and $f(\omega) = [\exp(\omega/T) + 1]^{-1}$ is the Fermi function. The Lagrange multiplier λ is absorbed into the renormalized impurity level energy, $\varepsilon \equiv \varepsilon_0 + \lambda$. The factor p in the

second term is $1/N_f$ in model I, while $p = 1$ in model II. Hence it is model II which generates a true large- N_f expansion, with all terms in the impurity free energy F_{imp} proportional to N_f .

From $H(0) < 0$, $H(\Delta^-) = +\infty$, and $dH/d\omega > 0$, we conclude that there is a unique solution to the equation $H(\omega) = 0$ on the interval $\omega \in [0, \Delta]$. Call this root Ω . We use the external field B as a Lagrange multiplier so that we may fix the total value of S^z . Making a Legendre transformation to $G_{\text{imp}}(S^z) = F_{\text{imp}}(B) - 2\mu_B B S^z$, with $S^z = -\frac{1}{2}, 0, +\frac{1}{2}$, we set $\partial F_{\text{imp}}/\partial(\mu_B B) = 0$, and obtain, at $T = 0$ (assuming $0 < \mu_B B < \Delta$),

$$G_{\text{imp}}^0/N_f = \varepsilon + p(\varepsilon - \varepsilon_0)(|b|^2 - r) + \mathcal{A} \quad (12)$$

$$\mathcal{A} = \frac{1}{\pi} \int_{\Delta}^{\omega_0} d\omega \text{Im} \ln H(\omega - i0^+) - \Omega \delta_{S^z,0}, \quad (13)$$

where $\omega_0 = \sqrt{W^2 + \Delta^2}$; W is the half-bandwidth in the electrodes. The mean field equations, obtained by setting $\partial G_{\text{imp}}^0/\partial|b|^2 = 0$ and $\partial G_{\text{imp}}^0/\partial\varepsilon = 0$ are

$$1 + p(|b|^2 - q) + \frac{\partial \mathcal{A}}{\partial \varepsilon} = 0 \quad (14)$$

$$p(\varepsilon - \varepsilon_0) + \frac{\partial \mathcal{A}}{\partial |b|^2} = 0, \quad (15)$$

and the Josephson current is

$$I = \frac{2e}{\hbar} \frac{\partial \mathcal{A}}{\partial \delta}. \quad (16)$$

Thus, for $0 \leq \mu_B B < \Omega$, the ground state has $S^z = 0$, while for $\Omega < |\mu_B B| < \Delta$, the ground state has $S^z = -\frac{1}{2} \text{sgn}(B)$.

For $p = r = 1$, we can show that the ground state energies satisfy $\Delta G_{\text{imp}}^0 \equiv G_{\text{imp}}^0 - G_{\text{imp}}^0 > 0$, which means that the mean field slave boson theory cannot describe the π or π' phases. The energy difference ΔG_{imp}^0 is minimized at $\delta = \pi$. The value of ΔG_{imp}^0 is an increasing function of the bare impurity level energy ε_0 . However, there are no solutions to the mean field equations for $\varepsilon_0 < \varepsilon_0^{\min} = -4\pi^{-1}\Gamma_a \cosh^{-1}(\omega_0/\Delta) - 2\Gamma_a \delta_{S^z,0}$. Rather, the endpoint solution $\varepsilon = |b|^2 = 0$ holds. Thus, the best we can do is $\Delta G_{\text{imp}}^0 = 0$, but in this case $G_{\text{imp}}^0 = \varepsilon_0$, independent of δ , and there is no Josephson current.

IV. LARGE Δ LIMIT

The case $\Delta \rightarrow \infty$ (with U finite) may be solved exactly. We begin with the Hamiltonian of eqn. (1), integrating out the fermion degrees of freedom in the superconductors [6]. This generates an induced action,

$$S_{\text{ind}} = \sum_{\omega_m} \bar{\Psi}_i(\omega_m) [\sigma^z \mathcal{G}(\omega_m) \sigma^z]_{ij} \Psi_j(\omega_m)$$

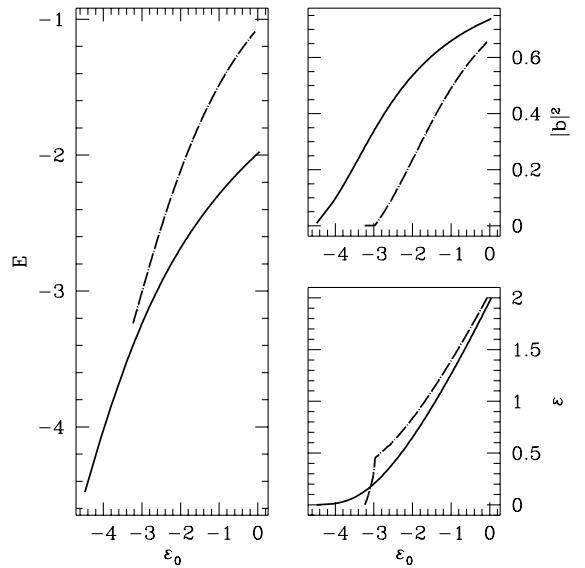


FIG. 3. Mean field parameters *versus* ε_0 . $\Delta = 1$, $\Gamma_a = 0.650$, $\Gamma_g = 0.630$, $B = 25$, $\delta = 0$, and $p = r = 1$. Solid curve is $S^z = 0$, dot-dash is $S^z = \pm\frac{1}{2}$.

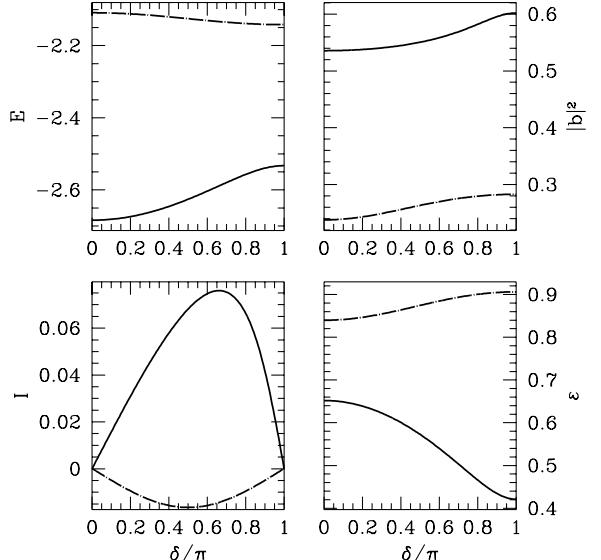


FIG. 4. Mean field parameters and Josephson current *versus* $\delta = 0$ for $\varepsilon_0 = -2$, $\Delta = 1$, $\Gamma_a = 0.650$, $\Gamma_g = 0.630$, $B = 25$, $\delta = 0$, $p = r = 1$. Solid curve is $S^z = 0$, dot-dash is $S^z = \pm\frac{1}{2}$.

$$\Psi(\omega_m) = \begin{pmatrix} c_{\uparrow}(\omega_m) \\ \bar{c}_{\downarrow}(-\omega_m) \end{pmatrix} \quad (17)$$

$$\mathcal{G}(\omega_m) = \sum_{\alpha} \frac{\Gamma_{\alpha}}{\sqrt{\omega_m^2 + \Delta_{\alpha}^2}} \begin{pmatrix} i\omega_m & \Delta e^{i\delta_{\alpha}} \\ \Delta e^{-i\delta_{\alpha}} & i\omega_m \end{pmatrix}.$$

If the dynamics all occur on frequency scales $\omega \ll \Delta$, we may ignore the Matsubara frequencies ω_m in comparison with Δ . Adding the induced action to the bare action

for the impurity, we find the resultant action is that for a Hamiltonian

$$\mathcal{H}_{\text{eff}} = \varepsilon_0(c_{\uparrow}^{\dagger}c_{\uparrow} + c_{\downarrow}^{\dagger}c_{\downarrow}) - \chi c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger} - \chi^* c_{\downarrow}c_{\uparrow} + Uc_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}c_{\downarrow}c_{\uparrow}, \quad (18)$$

where

$$\chi = \Gamma_L e^{i\delta_L} + \Gamma_R e^{i\delta_R}. \quad (19)$$

The ground state energy is $E_D^0 = \varepsilon_0$ for the Kramers doublet, and

$$E_S^0 = \varepsilon_0 + \frac{1}{2}U - \sqrt{(\varepsilon_0 + \frac{1}{2}U)^2 + |\chi|^2} \quad (20)$$

for the singlet. Thus, for $U < U_c$, where

$$U_c = 4\sqrt{\Gamma_a^2 - \Gamma_g^2 \sin^2(\frac{1}{2}\delta)}, \quad (21)$$

the Coulomb repulsion is too weak to overcome hybridization effects, and the ground state is a singlet for all ε_0 . For $U > U_c$, the ground state will be a doublet provided

$$-U - \sqrt{U^2 - U_c^2} < \varepsilon_0 < -U + \sqrt{U^2 - U_c^2}. \quad (22)$$

This allows the possibility of a level crossing as a function of δ if $E_s^0 < E_d^0 < E_s^0$. However, the doublet energy is independent of δ in this model, hence there is no Josephson coupling in the doublet ground state.

V. CONCLUSIONS

Using a generalization of the variational wavefunctions applied in the study of the Kondo effect [8,9], we have demonstrated that the $U = \infty$ interacting impurity Josephson junction exhibits a first order phase transition for $\Delta \approx T_K$. When $\Delta \lesssim T_K$, the ground state of the system is a singlet, and $E(\delta)$ is minimized at $\delta = 0$ and maximized at $\delta = \pi$. When $\Delta \gtrsim T_K$, the ground state is a Kramers doublet, the stability of $\delta = 0$ and $\delta = \pi$ is reversed, and the system forms a π -junction. For $\Delta \simeq T_K$, the singlet and doublet energy curves may cross, in which case the ground state energy has a kink as a function of δ [6] and is strongly nonsinusoidal.

We also solved for the junction's properties within a slave boson mean field theory. Unfortunately, this approach is unable to identify a phase transition, and the singlet state always is lower in energy than the doublet. One must go beyond the static mean field approach, as has recently been accomplished in ref. [7], to see the transition.

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